A Single-Crystal Model for High-strain-rate Applications

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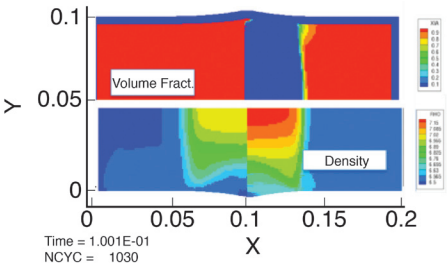
A thermodynamic framework is being used to model single-crystals for the extreme conditions of high-strain rate and high pressure. The effects of nonlinear elasticity, solid-solid phase transformations, plastic slip and twinning, and damage are included in the approach. The single-crystal model will be implemented into a structural analysis and used to pursue a polycrystal response. Coarse-graining or homogenization techniques will be considered in an effort to generate macro-mechanical models. The effort is closely coupled with experimental, microscopy, and diffraction studies.

*Fig. 1. Simulation of a plate impact experiment. Upper contour of volume fraction and lower contour of density (g/cm**3).*



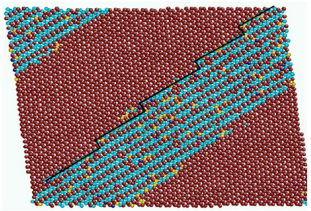


Fig. 2. Molecular dynamics simulation of shear on a Zr sample.

Predictive material models are necessary for the design and life extension of structures as well as the interpretation of subscale experimental investigations. Accurate models are required to provide deformation characteristics for a diverse range of loading scenarios. Predictive models are especially important for extreme conditions where experimental investigations cannot be conducted. To simulate component performance, increased burden is placed on modeling the effects of manufacturing processes on materials and on predicting their design behavior. In the past, uncertainty was mitigated with conservative designs. The macro-mechanical response of materials has its basis in the microstructure of the material. That is, deformation processes are dictated by mechanisms at the subgrain scale. The single-crystal or meso-mechanical length scale (the order of 50 μm) provides an intermediate length and time scale, which bridges the scales that are modeled using atomistic and macro-mechanical approaches.

The physics of solid-solid phase transformations has been addressed at many length scales. Molecular dynamics (MD) simulations have examined the effects of shear, hysteresis, and high-strain rates on the transformation process. Micro-mechanical models, which incorporate the details of nucleation, interface motion, and twin growth, have demonstrated the ability to describe the fundamental phenomena inherent to the transformation processes [1,2]. Meso-mechanical models have explored the details of phase transformations at the single-crystal scale [3-5]. However, few single-crystal approaches address the conditions, which are inherent to high-pressure and strain-rate phenomena [6,7]. Macro-mechanical approaches are necessary for addressing the deformation process of engineering structures. Macro-mechanical models do not, in general, address issues related to meta-stability, hysteresis, retained high-pressure phases, and the effects of shear on the transformation processes.

A model is being developed for the large deformation of single crystals under the conditions of high pressure and high-strain rate. The effects of deformational and transformational twinning, plastic slip, phase transformations, and damage are being considered. The model is not intended to resolve individual transformation interfaces or domains. Instead, volume fractions of the constituents within a representative volume of the material are modeled. Each constituent that is represented by a volume fraction is assumed to have the same material properties, such as lattice orientations, strain, and temperature. The constituents are also assumed to rotate together. A number of details are omitted in the model, including the nucleation of dislocations and damage. A thermodynamic framework, which is developed in terms of free energies, is used. In the model, the total deformation gradient (F) is divided into contributions due to elasticity (F^e), plasticity and damage (F^p), and the transformation process (F^ϕ):

$$F = F^e F^p F^\phi \tag{1}$$

The velocity gradient (L^p) of the plastic component is obtained using sums over slip (s) and deformation twin (t) systems:

$$L^p = \dot{F}^p F^{p-1} = \sum_s \dot{\gamma}^s \, (\vec{s}^s \otimes \vec{n}^s) + \sum_t \gamma^t \, (\vec{s}^t \otimes \vec{n}^t) \tag{2}$$

In Eq. (2), γ, $\vec{n}$, *and* $\vec{s}$ are the deformation resistance, slip or twin plane normal, and shear directions. The deformation gradient for the transformation process is obtained using sums over the transformation systems (ϕ):

$$\dot{F}^\phi = \sum_\phi \dot{\xi}^\phi \gamma^\phi (b^\phi \otimes m^\phi) \tag{3}$$

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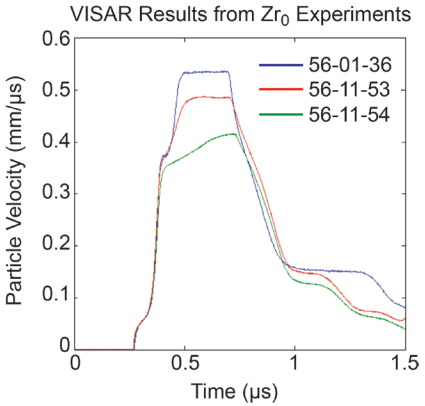
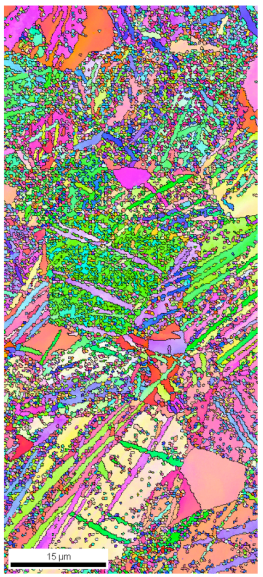


Fig. 3. Particle velocity measurements for recent plate impact experiments.

In Eq. (3) ξ^{ϕ}, γ^{ϕ}, *and* $\vec{m}^{\phi}$ are the mass fractions, shape strain, and normal to the transformation plane. Computational solutions of the resulting system of equations are obtained using an extension to existing approaches for single-crystal plasticity [8].

The driving force for phase transformations includes terms due to mechanical work, thermal energy, surface energy, and defect energy of the constituents. These forces will be extended to address the high strain-rate applications that are of interest. Although a general model formulation is being pursued, the α (hexagonal close packed) to ω (hexagonal) phase transformation in titanium (Ti) or zirconium (Zr) is being considered because of the plethora of experimental and atomistic information that is available for these elements. The model will allow the ability to include the effects of hysteresis, retained high-pressure phase, and kinetics of the transformation process.



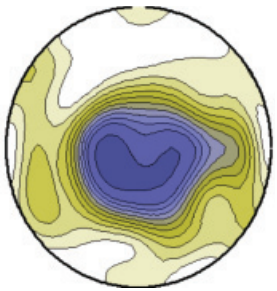


Fig. 4. Microscopy and diffraction results for a plate impact sample of Zr.

A plate impact simulation of Zr flyer ($0.0 < x < 0.1$ cm) and target ($0.1 < x < 0.2$ cm) plates is provided in Fig. 1, using a preliminary version of the proposed model. Each computational cell within the target plate of the simulation is assumed to be a single crystal. MD simulations (Fig. 2) have been used to explore the effects of shear and thermal cycling on the transformation process of Zr. Furthermore, MD simulations and experiments have been instrumental in defining material parameters for the single-crystal model. Polycrystal simulations will be used to pursue averaged quantities, which are necessary to explore improved macro-mechanical models for transformation processes. Coarse graining techniques also will be considered as a means to generate macro-mechanical models.

This effort is coupled to small-scale experimental investigations. Plate impact experiments have pursued the effects of peak pressure and temperature on the transformation process and meta-stability of Zr. Recently, two experiments were conducted at peak pressures of 8.0 GPa and 10.5 GPa (Fig. 3). The particle velocity response of the 8.0 GPa experiment indicated a sluggish transformation process relative to higher peak pressure experiments. Furthermore, whereas ~ 35% retained high-pressure (ω) phase was observed in past experiments, ~63% and ~82% retained high-pressure phase were observed in the 8.0 GPa and 10.5 GPa experiments, respectively. Diffraction investigations also suggest the presence of another crystalline structure. This result could provide insight into the potential pathway for the high-pressure transformation. Whether the transformation process is completed during the initial compression of the sample still is unknown. These results along with past torsion experiments, which resulted in ~95% retained high-pressure (ω) phase, suggest the importance of shear on the transformation process. Currently, the effects of shear and rate are not included in the existing phase transformation models that are used in engineering analyses. Future efforts will focus on microscopy (Fig. 4) and diffraction investigations of the plate impact samples. Information regarding the texture, transformation systems, and mechanical properties of the high-pressure phase will be considered.

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